RSFIT User's Guide

Quick start

RSFIT v3.4 and higher requires an input file. The syntax is

rsfit [-vef] [filename]

RSFIT must be run from a subdirectory called "input" or a directory called "output" with the same rank (that is, ../output). Both the input and output directories must exist. The input file in turn requires certain parameters for a fit to be performed. There are a substantial number of optional commands. At the minimum, one needs a file that contains roughly the following

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#Sample input file
#Required parameters

#OUTFILE <filename> specifies the name of the file where the final fit parameters,
#including all the limits, constraints, names of files, starting and final parameters, etc.,
#are to be stored.
OUTFILE sample

#STDDIR <run_directory> gives the run directory for the k-space standard files
STDDIR jan00

#STDFILE <filename> <rdist> gives the name of a standard file to be used for fitting,
#and the pair distance corresponding to that standard
STDFILE u_o2.38.f8 2.3802

#KRANGE rkmin rkmax rkwidth ikwt gives the minimum and maximum wave vector
#to be used in the Fourier transform, the width of the window function used the
#transform, and the k-weight to be used, eg. K^2:
KRANGE 2.5 13.5 0.3 2

RRANGE 1.2 3.5
FITDIR jan00
FITFILE 119b1
#Not required, but close!
PEAK 0.05 0.0 3.0 –5 0.0 0.0
#All fits must be signaled as "ready" with this:
STARTFIT
```

To fit with more peaks, add STDFILE commands. The format of the file is free-format in the sense that the order of the input is not important, except that the STDFILE lines must

be sequential. (The same is true of CONSTRAINT and NONLINEAR commands. See the appropriate section.) To perform another fit, simply add the desired lines after the last STARTFIT command. If a given command is not given in the new fit, the values from the previous fit are used. There are some caveats to adding fits, however. The most important is that the number of STDFILES must be the same as in the first fit specified in the file. Also, at this time, you must not have CONSTRAINT or NONLINEAR lines in the subsequent fits.

Standard output files to a "rsfit filename.x" (.x is a version number) command are

../input/filename.x+1
../output/filename.x
../output/filename.x.cor (if a correlation matrix is requested).

If a '-f' option is given on the command line, the actual fit will be output into three files with names like

datafile_peak.zzz.x	This is the final pair distribution function used
datafile_rspk.zzz.x	This is the actual fit
datafile_diff.zzz.x	This gives the fit residuals

Finally, the format of the output file is not for the faint-of-heart. To translate this file into a more readable form, from the ../output directory type

readxxo filename.x

which will output a file called read.zzz.x.

Command summaries

Overview

Syntax is rsfit [-OPTIONS] input_filename

Command line options are –v, -f and –e.

Required input file commands are STDDIR, STDFILE, KRANGE, RRANGE, OUTFILE, FITDIR, FITFILE, STARTFIT.

Starting values for pair parameters are set either with PEAK or with SIGMAS, RSHS, AMPS, E0S, C3S, C4S.

Commands that constrain various parameters include LIMITS, INCSIG, INCRSH, INCAMP, INCE0, INCC3, INCC4, E0SAME, SIGSAME, RSHSAME, AMPRSAME, NONLINEAR, and CONSTRAINT.

Commands to set how the error analysis is performed are CORREL, ERRTYPE, VARSERR, VARRERR, VARAERR, VAREERR, VARTERR, and VARFERR.

Commands for specifying I/O: ALLPATHSOUT

Other optional commands are DERIVWT, NODERIVWT, REMGAUS, LAMBDA, NOMFP, KDATA, RDATA, IWRIT, MAXITER.

Comment lines start with either a '*' or a '#'. Blank lines are allowed.

The order of the commands is not important, except STDFILE lines must be sequential, as must CONSTRAINT and NONLINEAR command lines. Also, if multiple fits are specied within an input file, the number of STDFILE lines must either be zero or the same as the last fit, and no CONSTRAINT or NONLINEAR lines can be specified. Other kinds of constraints, such as E0SAME and INCRSH may be specified.

Fits begin with a STARTFIT command; that is, all information up to the STARTFIT command is used, and information below such a command is used for the next fit.

Detailed summaries

Command line options

-v verbose output. Includes a continuously updated line with the number of calls to the EXAFS function routine, an updated R(%) and C2 (=chi2 with data errors taken as unity). The last two numbers on this line are a continuous update of C3 and C4.

-f output fit files. This flag MUST be present to obtain fit files.
-e perform error analysis. This flag MUST be present to perform error analysis.

Required commands

Parameters starting with 'i' are integers. All others are real or character strings.

KRANGE kmin, kmax, kwin, ikwt
Specifies range in k-space for the Fourier transform. kmin is the minimum and kmax is the maximum for the Gaussian window. kwin is a width for the Gaussian window. ikwt is the exponent in k^ikwt * chi(k) used for the transform, and thus for the fit.

RRANGE rmin, rmax
Specifies the range in r-space overwhich the statistical chi^2 will be calculated.

STDDIR run_directory
Specifies the run_directory where the standard files are stored. For instance, if the standard files are in a directory /home/exafs/exdata/jan00/ks (all standard files are stored in k-space), then run_directory is 'jan00'.

STDFILE filename, r_std
Specifies the filename of an EXAFS standard, together with the effective pair distance r_std of that standard.

FITDIR datafile_dir
Specifies the directory where the data files are stored. For instance, if the data files are in a directory /home/exafs/exdata/jan00/ks (data files are assumed to be in k-space unless an RDATA command is given), then datafile_dir is 'jan00'.

FITFILE datafile
Specifies the datafile filename to be fit.

STARTFIT
Command that signals RSFIT that all the input has been entered.

Parameter input

PEAK σ, Δr, A, ΔE0, C3, C4
Specifies starting parameters for a given atom pair. The number of the pair is given by the number of PEAK lines in the input file. So, for instance, if there are 5 standards, there should be 5 PEAK lines, the first one corresponding to the first standard, the 2nd PEAK line to the 2nd standard, etc. The starting parameters are the distribution width, σ (Å); the shift in pair distance from the standard's value, Δr (Å); a multiplicative coefficient A, the shift in E0, ΔE0 (eV); the third cumulant, C3 (Å); and the fourth

cumulant C4 (Å). All of these values are actually shifts from the corresponding standard file. If one uses a PEAK command, it is best not to use the SIGMAS, RSHS, AMPS, E0S, C3S, or C4S commands.

SIGMAS $\sigma_1, \sigma_2, \ldots, \sigma_{TOT}$
Specify the distribution width σ's (Å) for each standard pair 1-TOT.

RSHS $\Delta r_1, \Delta r_2, \ldots, \Delta r_{TOT}$
Specify the r-shifts (Å) for each standard pair 1-TOT.

AMPS $A_1, A_2, \ldots, A_{TOT}$
Specify the multiplicative coefficients *A* for each standard pair 1-TOT.

E0S $\Delta E0_1, \Delta E0_2, \ldots, \Delta E0_{TOT}$
Specify the E0 shifts (eV) for each standard pair 1-TOT.

C3S $C3_1, C3_2, \ldots, C3_{TOT}$
Specify the third cumulant C3's (Å) for each standard pair 1-TOT.

C4S $C4_1, C4_2, \ldots, C4_{TOT}$
Specify the third cumulant C4's (Å) for each standard pair 1-TOT.

Constraining commands

LIMITS sig_limit, rsh_limit, ampr_limit, e0_limit, c3_limit, c4_limit
Default is to not impose limits.

INCSIG sig_inc1, sig_inc2, …, sig_incTOT
Default values for all peaks is 0.01 Å.

INCRSH, INCAMP, INCC3, and INCC4 are similarly specified, with the same default values. INCE0 is similarly specified, but the default value is 1 eV.

E0SAME
Forces all E0 shifts for all standards to be the same.

SIGSAME
Forces all widths σ for all standards to be the same.

RSHSAME
Forces all pair distance shifts Δr for all standards to be the same.

AMPRSAME
Forces all amplitude ratios to be held fixed. For instance, if one uses a command

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AMPS 1.0 2.0
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for a 2-peak fit, AMPRSAME will keep the amplitude of the second peak to be twice that of the first peak. A possible result might be

AMPS 0.95 1.90

NONLINEAR Pfix, P1, P2, C1, C2, C3

This line specifies a nonlinear constraint. The P's indicate a parameter in the form Sx, Rx, Ax, Ex, Tx, and Fx for the σ, Δr, A, ΔE0, C3 or C4 parameter of the xth peak. For example, 'A3' is the parameter for the amplitude of the 3rd peak, and 'F19' is the fourth cumulant for the 19th peak. The constraint is in the form:

Pfix=C1*P1*P2 + C2*P1/P2 + C3

All NONLINEAR lines must precede any CONSTRAINT lines, and must be sequential in the input file. Also, NONLINEAR lines must only be specified in the first fit in an input file.

CONSTRAINT Pfix, P1, P2, C1, C2, C3

This line specifies a linear. The P's are described above under NONLINEAR. The constraint is in the form:

Pfix=C1*P1 + C2*P2 + C3

All CONSTRAINT lines must follow any NONLINEAR lines, and must be sequential in the input file. Also, CONSTRAINT lines must only be specified in the first fit in an input file.

Error analysis

ERRTYPE ierrtype, [data_sigmas]

Specifies whether errors are calculated in the positive direction (ierrtype=1), the negative direction (ierrtype=-1) or both (ierrtype=0). The default value is ierrtype=1. If data_sigmas are specified, these are used to calculate the real statistical chi^2 for determining the error bars on the fitted parameters. If data_sigmas are not specified, they will be estimated by using Stern's rule to give the number of independent parameters, then setting the final chi^2 equal to the degrees of freedom in the fit, with data_sigmas as the only variable.

VARSERR i1, i2, …, iTOT

Specifies which σ parameters will have their error bars calculated, where ix=0 indicates to not determine the error on the σ parameter for the ith peak, and ix=1 indicates to determine the error. Default values set all ix=1. Note that errors are only calculated is the parameter in question is varied in the fit.

VARRERR, VARAERR, VAREERR, VARTERR, and VARFERR commands specify same information for the other variable types.

I/O Handling

ALLPATHSOUT
If a –f flag is given, output all fit files, including the individual paths. The default is to not include the individual paths.

Miscellaneous commands

MAXITER imax_iterations
Sets the maximum number of calls to the EXAFS function routine. The default value is imax_iterations=3000. This is useful for not allowing a fit to go on and on and on and on…

LAMBDA mfp
Indicates to mfp (Å) as the mean-free path for the amplitude correction when applying r-shifts. The default value is 8.0 Å.

NOMFP
Turns off the default mean-free path correction.

NODERIVWT
Indicates not to use derivative weighting when calculating chi^2. This is the default.

DERIVWT
Turns on derivative weighting for calculating chi^2.

REMGAUS width
Indicates that negative values of fitted σ's are possible (not default)! This is often the case when using experimentally derived standards. In this case, width should be set as the maximum expected difference between the data and the standard, and should be a positive number. For low temperature experimental standards, width=4.0 Å is generally sufficient.

KDATA
Indicates data file is in k-space. This is the default.

RDATA
Indicates the data is in r-space. In this case KRANGE is not required. THIS OPTION HAS NOT BEEN TESTED!

IWRIT
Turns on some extra verbosity…